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A NEW OPTIMIZATION-BASED APPROACH TO IMPROVING GENERALIZATION IN MACHINE LEARNING HAS BEEN PROPOSED AND COMPUTATIONALLY VALIDATED ON SIMPLE LINEAR MODELS AS WELL AS ON HIGHLY NONLINEAR SYSTEMS SUCH AS NEURAL NETWORKS.

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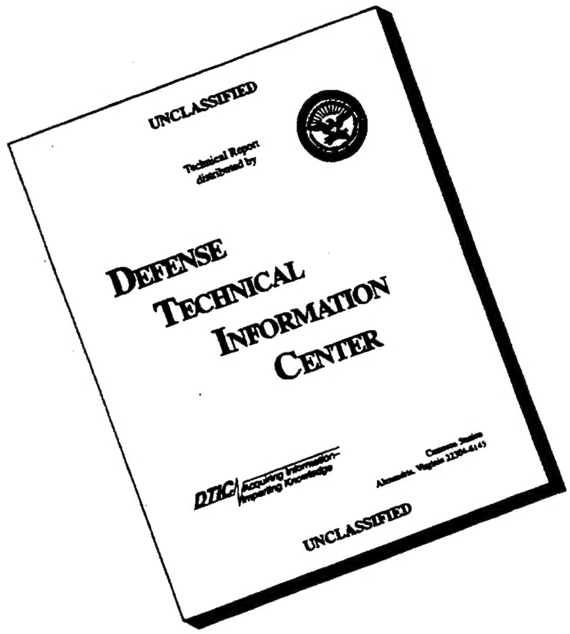

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RE: Final Report for F49620-94-1-0036

AFOSR GRANT F49620-94-1-0036
Final Technical Report

O. L. Mangasarian, R. R. Meyer & M. C. Ferris

Reporting Period: 11-01-93 to 10-31-95

A. Highlights

- 34 Papers published
- 14 Papers accepted for publication
- 14 Papers submitted for publication
- 8 Ph.D. Students Graduated
- 2 Meetings Organized
- 4 Technology Transfer Items
- Department of Energy Computational Science Award for "Breast Cancer Diagnosis via Linear Programming"

B. Research Results

1. Xcyt, our linear-programming breast cancer diagnostic-prognostic program, has been enhanced to give a 97.5% cross-validation diagnostic accuracy, and a 100% chronological diagnostic correctness over the last twenty four months on 176 consecutive patients.
2. A very effective bilinear programming approach has been proposed and implemented for the NP-complete general linear complementarity problem. Major iterations for the algorithm remained a constant equal to 4, for problem sizes between 10 and 3000.

3. A powerful smoothing approach to a very class wide of optimization and complementarity problems has been proposed and implemented. For mixed and other nonlinear complementarity problems, the smooth approach appears to outperform all currently available methods.

4. A novel mathematical programming approach to minimizing the number of misclassifications by a plane attempting to separate two point sets, has been proposed and implemented successfully. Although we have established that this is an NP-complete problem, our approach has successfully solved many real world problems.

5. A completely new optimization-based approach to improving generalization in machine learning has been proposed and computationally validated on simple linear models as well as on highly nonlinear systems such as neural networks.

6. First deterministic proof of convergence of the classical Backpropagation Algorithm for training neural networks has been given under precise and simple conditions. The proof covers parallel implementation as well as a momentum term.

7. A new broad class of complementarity problems, the extended linear complementarity problem, that subsumes most of the important classes has been defined. Existence results, error bounds and computational algorithms for this general class of problems have been given.

8. Until now, there had been no formulation of a fundamental problem of mathematical programming: the ill-posed linear complementarity problem. We have formulated a regularization of this problem as a linear program with equilibrium constraints, proved that the regularized problem always has a solution, and gave exact penalty methods for its solution as well as a parametric method.

9. A new mathematical programming formulation of the feature selection problem of machine learning has been formulated and coded. The new formulation readily detects noisy as well as insignificant features in a given problem and removes them. Test results on real world databases such as the Wisconsin Breast Cancer Database, identifies four important features out of nine. This results in a diagnostic separation based on four features that is as good as the one based on the original nine features.

10. Distributed high-level parallel genetic algorithms (GA's) were developed for minimum perimeter problems motivated by domain decomposition methods. This approach is based on the concept of stripe decomposition and rapidly produces feasible solutions within 0.1% of the theoretical lower bound for problems involving more than 1,000,000 binary variables. Comparison with standard graph partitioning approaches based on eigenvalue techniques demonstrated that the GA approach yielded solutions of significantly better quality and also was able to handle problems of sizes that were intractable for the eigenvalue method.

11. A knapsack-based method for optimal domain decomposition of certain classes of rectangular grids was devised and implemented. This technique is very fast and was able to produce provably optimal solutions to problems that would have more than one billion binary variables in a standard formulation.

12. Variable-penalty generalizations of alternating direction (ADI) methods were established. These techniques are very important for accelerating convergence of the ADI method. Computational implementations on the CM-5 supercomputer showed a one-to-two order of magnitude speedup relative to solution of structured large-scale problems using standard techniques.

13. A new relaxation method for convex network problems was developed that has the property of handling problems with ill-conditioned cost functions with the same excellent efficiency as well-conditioned nonlinear problems. An asynchronous convergence result has also been established for this method.

14. Massively parallel algorithms for extremely large quadratic programs were implemented on two parallel machines. Obstacle problems with over 9,000,000 variables were solved by this approach.

15. We continued to develop and extend the PATH solver (currently the fastest and most robust mixed complementarity problem (MCP) solver) to solve newly developed and formulated economic and engineering models. We implemented a preprocessor to determine the initial active set based on projected gradient and Newton methods for variational inequalities. Our implementation of these techniques can add and drop many constraints at a single iteration. This has proven significant on

a class of problems from optimal control. Nonmonotone and watchdog techniques have also been coded and extensively tested.

16. We extended the modeling language AMPL to have a complementarity link, similar to the link we developed to GAMS to enhance applicability of our PATH solver. This provides a bridge between the algorithmic designers and the problem modelers that enables modelers to use state of the art optimization techniques and algorithmic designers to test their methods on real life problems.

17. A survey paper by Ferris and Pang details all the currently known applications of complementarity. A large suite of these variational inequality problems have been formulated in our modeling environment to facilitate easy testing and comparison of algorithms for complementarity problems.

18. Many algorithmic developers are interested in testing their algorithms on models that arise from realistic applications, with reasonable size and real data. The Complementarity Toolbox that we have developed allows problem data from GAMS/MCP (the industry standard modeling format) to be used within MATLAB, a package for numeric computation and visualization. Several other researchers have used this interface since we made it publically available.

19. Several papers comparing this solver to other algorithms were written in this period. This survey identified the algorithms PATH and SMOOTH developed by CPO as the most effective solvers for the large class of problems that were tested.

20. Extensions to more complex models occurring in economics are now possible allowing formulation and solution using the tools developed during this grant. As an example of this, we performed work in the carbon emission field and making recommendations on the use of exemptions and grandfathered permits for the German government. Application work relating to traffic congestion modeled some complex routing problems in a complementarity format and solved these much quicker and more accurately than reported in the literature.

21. We devised a general pivotal technique for solving affine variational inequalities. Using this algorithm, notions of P_C matrices and copositive-plus normal equations were explored in a geometric setting. Significant

extensions to the existing convergence results were obtained. Interior point methods for such problems were also developed, along with new convergence results.

22. We implemented the NE/SQP algorithm for box constrained variational inequalities and showed it to be ineffective for many problems. A perturbation technique was devised to improve the robustness of this algorithm and implemented in the code QPCOMP. The perturbational idea greatly improved robustness and has since been incorporated into the PATH solver.

23. We have generalized the MCP format to include general polyhedral maximal monotone multifunctions as well as the normal cone operator. A class of algorithms has been develop and implemented for the solution of such problems with its major applications coming from general penalty theory.

24. We have explored the relationship of sharpness to local quadratic convergence of convex composite optimization algorithms. A general theory which allows one to prove local quadratic convergence of standard Newton–type algorithms applied to problems satisfying our sharpness condition has been developed.

25. We have used the Thinking Machines CM5 to enable real time visualization of volumes generated from slices of images formed using a confocal microscope. In a multidisciplinary approach involving members of the Center for Neuroscience and myself, the project sends raster files from the microscope over a FDDI link to the CM5. Specially adapted software written by Ferris and students is used to perform volume rendering. The resulting volumes are transferred back across the FDDI link to a Silicon Graphics Iris (SGI) computer which displays the image (in real time). The tool we have developed is now in use by members of the Center for Neuroscience.

C. Papers Published During Reporting Period

1. Z.-Q. Luo, O. L. Mangasarian, J. Ren & M. V. Solodov: "New error bounds for the linear complementarity problem", Mathematics of Operations Research 19(4), November 1994, 880-892.

2. O. L. Mangasarian & J. Ren: "New error bounds for the nonlinear complementarity problem", Communications on Applied Nonlinear Analysis 1, 1994, 49-56.

3. K. P. Bennett & O. L. Mangasarian: "Serial and parallel multicategory discrimination", SIAM Journal on Optimization, 4(4), November 1994, 722-734.

4. M. C. Ferris & O. L. Mangasarian: "Parallel variable distribution", SIAM Journal on Optimization, 4(4), November 1994, 815-832.

5. O. L. Mangasarian: "Misclassification minimization", Journal of Global Optimization 5(4), December 1994, 309-323.

6. O. L. Mangasarian & Jong-Shi Pang: "The extended linear complementarity problem", SIAM Journal on Matrix Analysis and Applications 16, January 1995, 359-368.

7. O. L. Mangasarian & M. V. Solodov: "Backpropagation convergence via deterministic nonmonotone perturbed minimization", in "Advances in Neural Information Processing Systems -6-", J. D. Cowan, G. Tesauro and J. Alspector, editors, Morgan Kaufmann, San Francisco, 1994, 383-390.

8. W. H. Wolberg, W. Nick Street & O. L. Mangasarian: "Machine learning techniques to diagnose breast cancer from image-processed nuclear features of fine needle aspirates", Cancer Letters 77, 1994, 163-171.

9. W. H. Wolberg, W. Nick Street & O. L. Mangasarian: "Image analysis and machine learning applied to breast cancer diagnosis and prognosis", Analytical and Quantitative Cytology and Histology 17, 1995, 77-87.

10. O. L. Mangasarian: "The linear complementarity problem as a separable bilinear program", Journal of Global Optimization 6, 1995, 153-161.

11. O. L. Mangasarian, W. Nick Street & W. H. Wolberg: "Breast cancer diagnosis and prognosis via linear programming", Operations Research, 43(4), July-August 1995, 570-577.

12. W. H. Wolberg, W. Nick Street, D. N. Heisey & O. L. Mangasarian: "Computer- derived nuclear features distinguish malignant from benign breast cytology", Human Pathology 26, 1995, 792-796.

13. W. H. Wolberg, W. Nick Street, D. N. Heisey & O. L. Mangasarian: "Computerized breast cancer diagnosis and prognosis from fine needle aspirates", Archives of Surgery 130, 1995, 511-516.

14. O. L. Mangasarian: "Optimization in Machine Learning", SIAG/OPT Views-and-News, No. 6, Spring 1995, 3-7.

15. W. H. Wolberg, W. Nick Street, D. N. Heisey & O. L. Mangasarian: "Computer- derived nuclear grade and breast cancer prognosis", Analytical and Quantitative Cytology and Histology 1995, 17, 257-264.

16. O. L. Mangasarian: "Parallel gradient distribution in unconstrained optimization", SIAM Journal on Control and Optimization 33(6), 1995, 1916-1925.

17. Chunhui Chen & O. L. Mangasarian: "Smoothing methods for convex inequalities and linear complementarity problems", Mathematical Programming 71, 1995, 51-69.

18. Chunhui Chen & O. L. Mangasarian: "A class of smoothing functions for nonlinear and mixed complementarity problems", Computational Optimization and Applications 5, 1996, 97-138.

19. R.R. Meyer and J. Yackel: "Large-Scale Diversity Minimization via Parallel Genetic Algorithms", in *Large-Scale Optimization: State of the Art* , W.W. Hager, et al., eds., Kluwer Publishing, 1994.

20. R. De Leone, S. Kontogiorgis, R.R. Meyer, A. Zakarian, and G. Zakeri) "Coordination in Coarse-Grained Decomposition", SIOPT , 4, 777-793, 1994.

21. M. C. Ferris. Parallel constraint distribution for convex quadratic programs. *Mathematics of Operations Research*, 19:645–658, 1994.

22. E. J. Anderson and M. C. Ferris. Genetic algorithms for combinatorial optimization: The assembly line balancing problem. *ORSA Journal on Computing*, 6:161–173, 1994.

23. J. V. Burke and M. C. Ferris. Weak sharp minima in mathematical programming. *SIAM Journal on Control and Optimization*, 31:1340–1359, 1993.

24. M. Cao and M. C. Ferris. An interior point algorithm for monotone affine variational inequalities. *Journal of Optimization Theory and Applications*, 83:269–283, 1994.

25. M. C. Ferris and S. Lucidi. Nonmonotone stabilization methods for nonlinear equations. *Journal of Optimization Theory and Applications*, 81:53–71, 1994.

26. J. V. Burke and M. C. Ferris. A Gauss–Newton method for convex composite optimization. *Mathematical Programming, forthcoming*, 1995.

27. S. P. Dirkse and M. C. Ferris. The PATH solver: A non-monotone stabilization scheme for mixed complementarity problems. *Optimization Methods and Software*, 5:123–156, 1995.

28. M. C. Ferris and J. S. Pang. Nondegenerate solutions and related concepts in affine variational inequalities. *SIAM Journal on Control and Optimization*, 34:244-263, 1996.

29. S. P. Dirkse and M. C. Ferris. MCPLIB: A collection of nonlinear mixed complementarity problems. *Optimization Methods and Software*, 5:319–345, 1995.

30. M. Cao and M. C. Ferris. Lineality removal for copositive–plus normal maps. *Communications on Applied Nonlinear Analysis*, 2:1–10, 1995.

31. M. C. Ferris and D. Ralph. Projected gradient methods for nonlinear complementarity problems via normal maps. In D. Du, L. Qi, and R. Womersley, editors, *Recent Advances in Nonsmooth Optimization*, pages 57–87. World Scientific Publishers, 1995.

32. C. Böhringer, M. C. Ferris, and T. F. Rutherford. Exemptions, grandfathered permits and the costs of emission restrictions: Results from a general equilibrium model for six EU countries. In *Economic Aspects of Environmental Policy Making in a Federal System*, 1995.

33. M. C. Ferris and O. L. Mangasarian. Breast cancer diagnosis via linear programming. *IEEE Computational Science and Engineering*, 2:70–71, 1995.

34. M. C. Ferris and J. S. Pang. Report on First International Conference on Complementarity Problems. *IEEE Computational Science and Engineering*, 2(4):90, 1995. (Also appeared in *Optima*, 48:10.)

D. Papers Accepted for Publication During Reporting Period

1. W. Nick Street, O. L. Mangasarian & W. H. Wolberg: "An Inductive Learning Approach to Prognostic Prediction", in "Machine Learning: Proceedings of the Twelfth International Conference", A. Prieditis and S. Russell (editors), Morgan Kaufmann, San Francisco 1995, to appear.

2. Chunhui Chen & O. L. Mangasarian: "Hybrid misclassification minimization", Mathematical Programming Technical Report 95-05, February-July 1995, Advances in Computational Mathematics, to appear.

3. O. L. Mangasarian: "Mathematical programming in machine learning", Mathematical Programming Technical Report 95-06, April-July 1995, Proceedings of Nonlinear Optimization and Applications Workshop, Erice, June 1995, Plenum Press, to appear.

4. O. L. Mangasarian: "Machine learning via polyhedral concave minimization", University of Wisconsin, Computer Sciences Department, Mathematical Programming Technical Report 95-20, November 1995, "Applied Mathematics and Parallel Computing – Festschrift for Klaus Ritter", H. Fischer, B. Riedmueller, S. Schaeffler, editors, Physica-Verlag, Germany 1996, 175-188.

5. R. De Leone, R.R. Meyer and S. Kontogiorgis: "Alternating Direction Splittings for Block-Angular Parallel Optimization", Computer Sciences Department Technical Report 1217, to appear in *Journal of Optimization and Applications*.

6. J. Yackel, R.R. Meyer and I. Christou: "Minimum-Perimeter Domain Assignment", to appear in *Mathematical Programming*, 1996.

7. I. Christou and R.R. Meyer: "Optimal and Asymptotically Optimal Equi-Partition of Rectangular Domains via Stripe Decomposition ", "Applied Mathematics and Parallel Computing – Festschrift for Klaus Ritter", H. Fischer, B. Riedmueller, S. Schaeffler, editors, Physica-Verlag, Germany 1996, 77-96.

8. I. Christou and R.R. Meyer: "Optimal Equi-Partition of Rectangular Domains for Parallel Computation ", *Journal of Global Optimization*, 8, 15-34, 1996.

9. M. Cao and M. C. Ferris. A pivotal method for affine variational inequalities. *Mathematics of Operations Research, forthcoming*, 1996.

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13. M. C. Ferris, S. Lucidi, and M. Roma. Nonmonotone curvilinear stabilization techniques for unconstrained optimization. *Computational Optimization and Applications, forthcoming*, 1995.

14. M. C. Ferris and T. F. Rutherford. Accessing realistic complementarity problems within Matlab. In G. Di Pillo and F. Giannessi, editors, *Proceedings of Nonlinear Optimization and Applications Workshop, Erice June 1995*, New York, 1996. Plenum Press.

E. Papers Submitted for Publication During Reporting Period

1. W. Nick Street & O. L. Mangasarian: "Improved Generalization via Tolerant Training", Mathematical Programming Technical Report 95-11, July 1995, Machine Learning, submitted.

2. O. L. Mangasarian: "The Ill-Posed Linear Complementarity problem", Mathematical Programming Technical Report 95-15, August 1995, SIAM Proceedings of the International Conference on Complementarity Problems, The Johns Hopkins University, November 1-4, 1995, submitted.

3. P. S. Bradley, O. L. Mangasarian & W. Nick Street: "Feature selection via mathematical programming", University of Wisconsin, Computer Sciences Department, Mathematical Programming Technical Report 95-20, December 1995, ORSA Journal on Computing, submitted.

4. S. Kontogiorgis and R.R. Meyer: "A Variable-Penalty Alternating Directions Method for Convex Optimization ", submitted to *Mathematical Programming*, 1995.

5. R. De Leone, R.R. Meyer and A. Zakarian: "An ϵ-Relaxation Algorithm for Convex Network Flow Problems ", Center for Parallel Optimization Technical Report 95-02, submitted for publication, Operations Research.

6. Wayne Martin: "Fast Equi-Partitioning of Rectangular Domains Using Stripe Decomposition", Mathematical Programming Technical Report 96-2, submitted to Discrete Applied Mathematics.

7. M. C. Ferris and J. D. Horn. Partitioning mathematical programs for parallel solution. Technical Report 1232, Computer Sciences Department, University of Wisconsin, Madison, Wisconsin, May 1994, submitted to Mathematical Programming.

8. S. C. Billups and M. C. Ferris. Solutions to affine generalized equations using proximal mappings. Mathematical Programming Technical Report 94–15, Computer Sciences Department, University of Wisconsin, Madison, Wisconsin, 1994, submitted to Mathematics of Operations Research.

9. J. Eckstein and M. C. Ferris. Operator splitting methods for monotone affine variational inequalities, with a parallel application to optimal control. Mathematical Programming Technical Report 94-17, Computer Sciences Department, University of Wisconsin, Madison, Wisconsin, 1994, submitted to ORSA Journal on Computing.

10. M. C. Ferris, A. Meeraus, and T. F. Rutherford. Computing Wardropian equilibrium in a complementarity framework. Mathematical Programming Technical Report 95-03, Computer Sciences Department, University of Wisconsin, Madison, Wisconsin, 1995, submitted to Operations Research.

11. M. C. Ferris and J. S. Pang. Engineering and economic applications of complementarity problems. Discussion Papers in Economics 95–4, Department of Economics, University of Colorado, Boulder, Colorado, 1995, submitted to SIAM Review.

12. S. C. Billups and M. C. Ferris. QPCOMP: A quadratic program based solver for mixed complementarity problems. Mathematical Programming Technical Report 95–09, Computer Sciences Department, University of Wisconsin, Madison, Wisconsin, 1995, submitted to Mathematical Programming.

13. S. C. Billups, S. P. Dirkse, and M. C. Ferris. A comparison of algorithms for large scale mixed complementarity problems. UCD/CCM Report 67, Center for Computational Mathematics, University of Colorado at Denver, Denver, Colorado, 1995, submitted to Computational Optimization and Applications.

14. S. P. Dirkse and M. C. Ferris. Preprocessing techniques for large-scale complementarity problems. Mathematical Programming Technical Report 95-22, Computer Sciences Department, University of Wisconsin, Madison, Wisconsin, 1995, submitted to SIAM Proceedings of the International Conference on Complementarity Problems, The Johns Hopkins University, November 1-4, 1995.

G. Ph.D. Students Graduated During Reporting Period

1. W. Nick Street: "Cancer Diagnosis and Prognosis via Linear-Programming-Based Machine Learning", August 1994.

2. Michael V. Solodov: "Nonmonotone and Perturbed Optimization", August 1995.

3. Chunhui Chen: "Smoothing Methods in Mathematical Programming", August 1995.

4. Spyridon A. Kontogiorgis: " Alternating Directions Methods for the Parallel Solution of Large-Scale Block-Structured Optimization Problems", June 1994.
5. Golbon Zakeri: " Multi-Coordination Methods for Parallel Solution of Block-Angular Programs", May 1995.
6. Menglin Cao: Piecewise Linear Homotopies and Affine Variational Inequalities, January 1994.
7. Steven Dirkse: Robust Solution of Mixed Complementarity Problems, August 1994.
8. Stephen Billups: Algorithms for Complementarity Problems and Generalized Equations, August 1995.

H. Meetings organized

1. Ferris co-organized (with T. Rutherford, U. Colorado) a workshop on "Computational Methods for Dynamic Models of Uncertainty", at the University of Colorado-Boulder in March 1995. 20 researchers with interests in economics and complementarity attended.
2. In conjunction with J.S Pang, Ferris organized the "International Conference on Complementarity Problems" at Johns Hopkins University in November 1995. The meeting was attended by over 50 researchers in the area from over 20 countries; a report can be found on CPNET.

I. Technology Transfers

1. Xcyt, our linear-programming breast cancer diagnostic-prognostic program, is in current use at University of Wisconsin Hospitals for diagnosing and predicting recurrence of breast cancer, one of the deadliest diseases among women. Plans for use at other domestic and foreign institutions are under way.
2. The release of PATH as a GAMS subsystem has increased the visibility of the work of CPO and added many new users of this code (36 versions of the code purchased, and over 60 evaluation systems in use after 4 months).

3. In order to generate closer ties between the user community and algorithmic developers, we established (and maintain) CPNET, a WEB page for complementarity research. Further details of the work of CPO and other work in the complementarity area can be found on this site (http://www.cs.wisc.edu/cpnet/).

4. We created publically available tools that help algorithmic development for real-life applications of complementarity. We have created the basic complementarity toolbox for MATLAB, and other interfaces between problem solvers and algorithm developers. MCPLIB, the standard library of test problems for complementarity, the MATLAB interface and a MATLAB version of PATH are part of this toolbox.

J. Award

Awarded jointly with Michael C. Ferris on September 16, 1995, the Department of Energy Computational Science Award of $1,000, for the student project: "Breast Cancer Diagnosis via Linear Programming". This project, based on my cancer research, is available on the World Wide Web from: ftp://ftp.cs.wisc.edu/math-prog/teaching/, and has been widely accessed.